THIRD-GENERATION THERMODYNAMIC DESCRIPTION OF SiO$_2$

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Modern assessments of thermodynamic properties of elements and substances require more physically based models that provide accurate and reliable predictions in a wide range of temperatures from 0 K to temperatures above the melting point. In the present work the extended Einsten model [1] and the two-state model [2] were used to describe thermodynamic properties of silicon dioxide. The extended Einstein model, which includes harmonic vibrations into the heat capacity, was used for the thermodynamic description of α— and β—quartz and α— and β—cristobalite. The two-state model that assumes a liquid phase to consist of two kinds of atoms was used to describe the amorphous and liquid SiO$_2$, which were treated as the same phase. The optimization of the model parameters was based on the critical review of the experimental thermodynamic data available for SiO$_2$ and was carried out using ThermoCalc software [3]. In a number of studies the two-state liquid model was applied for thermodynamic description of the pure elements (e.g. metals). However, a rather limited data on the heat capacity of the supercooled liquid phase available for pure metals makes it difficult or even impossible to evaluate consistency of the calculated results with the experimental data. It should be pointed out that application of the model for the thermodynamic description of oxide melts (e.g. pure SiO$_2$) with extensive experimental data available for both the amorphous and supercooled liquid states has not yet been carried out and therefore is a challenging task. The thermodynamic assessment presented in this work provides a good description and high reproducibility of the low-temperature and high-temperature heat-capacity data and is consistent with the standard S$_{298}$ and enthalpy increment data.

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